Second Quantization and Bogoliubov Approximation

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Abstract

Recent experiments with trapped alkali atoms [3] have drawn enormous interest to the theoretical studies concerning Bose-Einstein condensation. The purpose of this paper is to review one of the approaches to study bosonic matter at zero temperature, namely the Bogoliubov approximation. Review of a necessary tool, the second quantization, will also be made.

1 Introduction

In 1925, Albert Einstein, by generalizing Satyendra Nath Bose's work [1] on photons, concluded [2] that macroscopic numbers of integer spinned atoms can collapse into one single quantum state if they are cooled to temperatures very close to the absolute zero. However, because of technical limitations of trapping technology, this phenomenon, known as Bose-Einstein Condensation (BEC), has not been observed until 1995, when more than one research group almost simultaneously managed to obtain BECs using trapped alkali atoms [3].

A common point of all these experiments is that they worked with weakly interacting atoms. The Bogoliubov approximation, which has long been known to theorists, provides a proper means to approach such systems. Although it is completely valid only at absolute zero temperature, it still gives admissible results in the temperature ranges concerned in the experiments.

The purpose of this paper is to review the Bogoliubov approximation. An essential tool to accomplish this is the *second quantization*, which is an extension of ordinary quantum mechanics. In part 2, it will be thoroughly studied. Bogoliubov approximation will be discussed in the third part.

2 Second Quantization

Second quantization is a powerful tool. First introduced by Jordan, Klein and Wigner in 1928 [4], it is now covered in many text books [5][6]. It can be used for field quantization, which makes it more powerful than the 'ordinary' quantum mechanics, that is the 'first quantization'. It can also be used to study the properties of many particle systems. Although it does not say anything more than the first quantization for that purpose, it introduces convenience. This is the reason that we will use it to approach Bose-Einstein Condensation.

Let us consider a specific and useful example rather than considering the most general case. Harmonic potentials are very common in physics and therefore familiar to physicists. Furthermore, to first approximation, every potential is harmonic around its equilibrium point. Also, in 1D there is no degeneracy and energy levels take the simple form $E_n = \hbar\omega(n+\frac{1}{2})$. Therefore, we choose to study a harmonic potential. The Hamiltonian of a system of N indistinguishable particles confined in a 1D harmonic trap is given as

$$H = \sum_{k=1}^{N} (-\frac{\hbar^2}{2m}\nabla_k^2 + m\omega^2 r_k^2) + \frac{1}{2}\sum_{k,l=1;k\neq l}^{N} V(r_k - r_l). \tag{1}$$

We will assume an interparticle potential of the form

$$V(r_k - r_l) = g\delta(r_k - r_l). \tag{2}$$

In general, the N-body wave function $\Psi(r_1, r_2, ..., r_N, t)$ can be written as a superposition of products of one body stationary wave functions $\phi_k(r_i)$:

$$\Psi(r_1, r_2, ..., r_N, t) = \sum_{k_1, k_2, ..., k_N} C(k_1, k_2, ..., k_N, t) \cdot \phi_{k_1}(r_1) \cdot \phi_{k_2}(r_2) ... \cdot \phi_{k_N}(r_N) \tag{3}$$

According to postulates of quantum mechanics, all existing particles can be divided into two subgroups: *fermions*, which are the particles with half-integer spin, and *bosons*, which are the ones with integer spin. The wave function of a system consisting of identical bosons must be symmetric with respect to the exchange of two particles, whereas that of a system consisting of fermions must be anti-symmetric. Mathematically stated, this implies

$$\Psi(..., r_i, ..., r_j, ..., t) = \Psi(..., r_j, ..., r_i, ..., t) \tag{4}$$

for bosons and

$$\Psi(..., r_i, ..., r_j, ..., t) = -\Psi(..., r_j, ..., r_i, ..., t) \tag{5}$$

for fermions. Since Bose-Einstein condensation occurs only in systems of identical bosons, fermionic systems will henceforth be omitted from this paper and unless otherwise stated, the equations will be valid only for bosons.

This is a natural point to raise the question "How many different states may exist with n_1 particles having the lowest energy E_1, n_2 particles having E_2, etc.?" It is not very hard to see (yet not obvious either) that for bosons (and also for fermions) the symmetry (anti-symmetry) condition precludes all but one such state for a given set of occupation numbers $n_1, n_2, ..., n_N$. That is to say, the occupation numbers n_i determine the wave function uniquely. This fact is due to the indistinguishability of the particles. In fact, if there could be more than one state with the same occupation numbers, this would be in contradiction with the indistinguishability.

As the occupation numbers define the wave function uniquely, it is possible to span the space by vectors defined by the occupation numbers. The space spanned by states of definite occupation numbers is called the Fock space. A typical vector in the Fock space is denoted by $|n_1 n_2 ... n_i ...\rangle$ which means that there are n_1 particles with E_1 etc.. Note that here i can be any integer regardless of the total particle number, so long as there is no restriction in the highest energy that a particle can have, even though there are a finite number of particles in the system.

Annihilation and creation operators for each of the energy eigenstates can be defined similarly to those encountered in the harmonic oscillator problems.

$\hat{b}_i^\dagger$ is defined as the operator that creates a particle in the E_i energy eigenstate, that is,

$$\hat{b}_i^\dagger|n_1 n_2 ... n_i ...\rangle = \sqrt{n_i + 1}|n_1 n_2 ...(n_i + 1)...\rangle. \tag{6}$$

The algebra of these operators is similar to that of harmonic oscillator operators, with some additions to define commutators of operators belonging to different modes:

$$\hat{b}_i|n_1 n_2 ... n_i ...\rangle = \sqrt{n_i}|n_1 n_2 ...(n_i - 1)...\rangle \tag{7}$$

$$[\hat{b}_i, \hat{b}_j] = 0 \tag{8}$$

$$[\hat{b}_i^\dagger, \hat{b}_j^\dagger] = 0 \tag{9}$$

$$[\hat{b}_i, \hat{b}_j^\dagger] = \delta_{ij} \tag{10}$$

The relationship between second quantization and ordinary quantum mechanics can be established once we define the *field operators*:

$$\hat{\psi}(r,t) = \sum_n b_n \phi_n(r) \tag{11}$$

$$\hat{\psi}^\dagger(r,t) = \sum_n b_n^\dagger \phi_n^*(r) \tag{12}$$

It is not hard to prove that given the orthonormality of the basis states, the field operator $\hat{\psi}(x,t)$ acting on the vacuum state $|0,0,...,0,...\rangle$ creates a particle at position x at time t. (At this point, the reader is urged not to confuse the vacuum state, which has no particles at all, with $|N, 0, ..., 0, ...\rangle$, the ground state of a system of N particles.) Similarly, the expression $\int f(x)\hat{\psi}(x,t)dx$ creates a particle with wave function $f(x)$. (Note that as $\int \phi_k(x)\hat{\psi}(x,t)dx$ creates a particle in the k^{th} eigenstate, it can be proven to be equal to $\hat{b}_k$.)

The commutators of field operators are also important:

$$[\hat{\psi}(r,t), \hat{\psi}(r',t)] = 0 \tag{13}$$

$$[\hat{\psi}^\dagger(r,t), \hat{\psi}^\dagger(r',t)] = 0 \tag{14}$$

$$[\hat{\psi}(r,t), \hat{\psi}^\dagger(r',t)] = \delta_{rr'} \tag{15}$$

The second quantized Hamiltonian $\hat{H}$ follows from the expectation value of H with the field operators. The one particle part of it becomes:

$$\hat{H}_0 = \int dx \hat{\psi}^\dagger(x,t)[-\frac{\hbar^2}{2m}\nabla^2 + m\omega^2 x^2]\hat{\psi}(x,t). \tag{16}$$

Some tedious but straightforward algebra is sufficient to show that

$$\hat{H}_0 = \sum_n E_n \hat{b}_n^\dagger \hat{b}_n. \tag{17}$$

Two particle operators are more tedious to handle, since their second quantized forms are given [5] by

$$\hat{V} = \frac{1}{2}\int\int drdr' \hat{\psi}^\dagger(r)\hat{\psi}^\dagger(r')V(r,r')\hat{\psi}(r')\hat{\psi}(r') \tag{18}$$

However, the the assumed Dirac delta form of the interparticle potential allows us to reduce the double integral into a single one:

$$\hat{V} = \frac{g}{2}\int dr\hat{\psi}^{\dagger}(r)\hat{\psi}^{\dagger}(r')\hat{\psi}(r')\hat{\psi}(r') \tag{19}$$

Although what is covered here is only a small part of the second quantization, these expressions give us enough facilities to consider the Bogoliubov approximation.

3 Bogoliubov Approximation

Bose-Einstein condensation occurs when the macroscoping majority of particles fall into the ground state, that is when the number of particles in the ground state, n_0, is $n_0 \approx N$ and therefore, $n_i/N \ll 1$ for $i \neq 0$. Therefore, it may prove to be convenient to write the field operator as

$$\hat{\psi}(r) = \phi_0(r)\hat{b}_0 + \sum_{i=1}^{\infty}\phi_i(r)\hat{b}_i. \tag{20}$$

Considering the fact that $|\hat{b}_i|...n_i...\rangle| \sim n_i$, the second term in this expression may be considered to be a small fluctuation:

$$\hat{\psi}(r) = \phi_0(r)\hat{b}_0 + \delta\hat{\psi}(r,t). \tag{21}$$

The validity of this approach can be questioned, since depending on the temperature the fluctuation part may become large and cannot be assumed to be small anymore. However, for Bose-Einstein condensation to occur, the temperature ranges considered should be very close to the absolute zero; hence, this approach is quite valid - though not flawless.

Now let us see the effect of the ground state annihilation operator $\hat{b}_0$ on the Bose-Einstein condensed state:

$$\hat{b}_0|n_0, ...\rangle = \sqrt{n_0}|n_0 - 1, ...\rangle. \tag{22}$$

But as we talk of *macroscopic* number of bosons in the ground state, the difference between n_0 and $n_0 - 1$ is negligible in the sense that $(n_0 - 1) - n_0 \simeq 1$ and hence we can assume

$$\hat{b}_0|n_0, ...\rangle = \sqrt{n_0}|n_0, ...\rangle. \tag{23}$$

So, the sole effect of the ground state annihilation operator is to multiply the state with the real number n_0. The idea behind Bogoliubov's approximation is to replace this operator $\hat{b}$ (and also its conjugate $\hat{b}^\dagger$) with the real number $\sqrt{n_0}$:

$$\hat{b}_0 \to \sqrt{n_0}. \tag{24}$$

$$\hat{b}_0^\dagger \to \sqrt{n_0}. \tag{25}$$

Hence, we obtain a field operator which differs from the stationary ground state wave function only by a small fluctuation part:

$$\hat{\psi}(r) = \sqrt{n_0}\phi_0(r) + \delta\hat{\psi}(r,t). \tag{26}$$

This completes our review. The second quantized Hamiltonian will be much easier to calculate when the field operator is used in this format, as the commutators will take simpler forms. Since $\delta\hat{\psi}(r,t)$ is assumed to be small, terms which are higher order with respect to it may be neglected. Omitting 3^{rd} and 4^{th} orders and choosing a ground state wave function which makes 1^{st} order terms vanish is a common approach [7].

A References

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